



chain nodes :

21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 61 63

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 42 43 44 45 46 47
48 49 50 51 52 53

chain bonds :

2-28 4-25 7-26 14-27 15-17 17-29 18-21 19-22 20-23 20-30 23-24 25-26 25-63 31-32
33-34 33-35 36-37 38-39 38-40 41-43

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-13 6-15 7-8 7-12 8-9 9-10 10-11 11-12 13-14 14-15
16-17 16-20 17-18 18-19 19-20 42-43 42-47 43-44 44-45 45-46 46-47 48-49 48-53
49-50 50-51 51-52 52-53

exact/norm bonds :

4-25 5-13 6-15 13-14 14-15 15-17 16-17 16-20 17-18 18-19 18-21 19-20 19-22 33-34
41-43

exact bonds :

2-28 7-26 14-27 17-29 20-23 20-30 23-24 25-26 25-63 31-32 33-35 36-37 38-39 38-40

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 42-43 42-47 43-44 44-45
45-46 46-47 48-49 48-53 49-50 50-51 51-52 52-53

G1:[*1],[*2],[*3],[*4],[*5],[*6]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS
40:CLASS 41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom
50:Atom 51:Atom 52:Atom 53:Atom 61:CLASS 62:Atom 63:CLASS